Supporting Information

Design of Covalent Organic Frameworks for Methane Storage

Jose L. Mendoza-Cortes[1], Tod A. Pascal[1], William A. Goddard III[*,1]

[1]Materials and Process Simulation Center (MC 139-74), California Institute of Technology, Pasadena, California 91125, USA,

E-mail: wag@wag.caltech.edu

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1 New COFs

Previous studies showed that the main topologies to be obtained given a connectivity of the three and four points of extension are **ctn** and **bor** [1],[2],[3], we designed new COFs with these characteristics but with different ligands. The proposed chemistry is same; condensation of boronic acids to give boroxine esters and borosilicates. The building blocks are shown in Figure S1 while the inset shows the type of condensations used.

2 Delivery amount

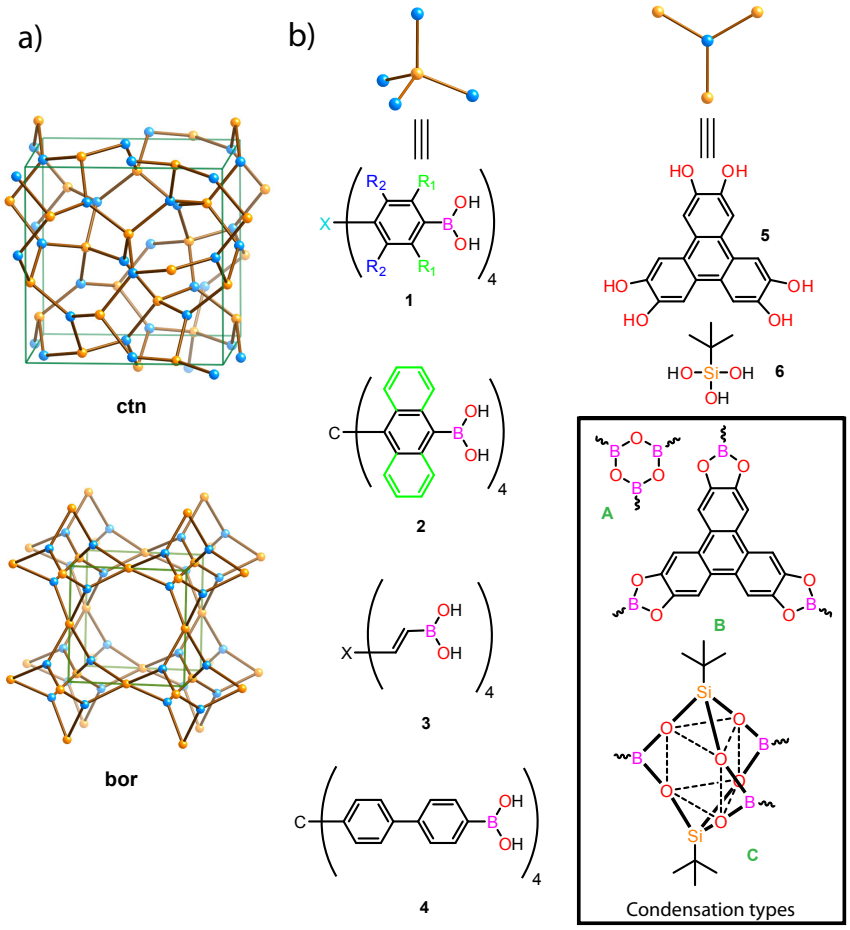
We have calculated v(CH_4 STP) v^{-1} delivery amount with respect to total volume of the framework. Here STP is the volume of methane at standard and pressure condition (STP; T = 298 K and P = 1.01 bar). In addition to the newly designed COFs, we have calculated the uptake amount of methane at room temperature from 0-300 bar for pusblished COFs [2],[4] as well as for MOF-177 [5] and MOF-200 [6].

2.1 1 to 100 bar

We have calculated the methane delivery amount from 1 to 300 bar, and the results are shown in Figure S2. This is the theoretical upper limit for methane to be delivered if no kinetic affects are taken into account.

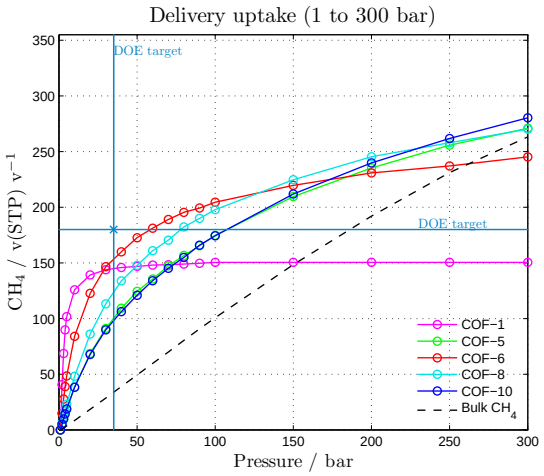
2.2 5 to 100 bar

We have calculated the methane delivery amount from 5 to 300 bar, and the results are shown in Figure S3. We have used 5 bar instead of 1 bar here in order to take into account possible kinetic effects. However, with this constraint we can see that none of the compounds presented in this work reach the DOE target. Also at 300 bar, COF-102-Ant performs worse than bulk methane.

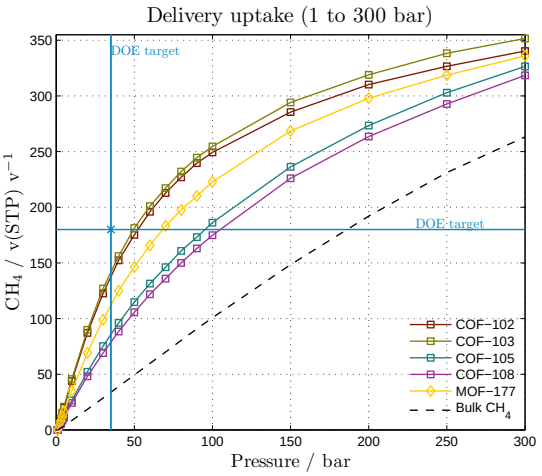


Reactants	Type		R_1	R_2	Name	topology
1	A	X=C	—H	—H	COF-102	**ctn**
1	A	X=C	$-CH_2CH_3$	—H	COF-102-Et-H	**ctn**
1	A	X=C	$-CH(CH_3)_2$	—H	COF-102-iPr-H	**ctn**
1	A	X=C	$-(CH_2)_2CH_3$	—H	COF-102-Pr-H	**ctn**
1	A	X=C	$-C(CH_3)_3$	—H	COF-102-tBu-H	**ctn**
1	A	X=C	$-CH_3$	$-CH_3$	COF-102-Me-Me	**ctn**
1	A	X=Si	$-CH_3$	$-CH_3$	COF-103-Me-Me	**ctn**
2	A	X=C	N/A	N/A	COF-102-Ant	**ctn**
3	A	X=C	N/A	N/A	COF-102-Eth-cis	**ctn**
3	A	X=Si	N/A	N/A	COF-103-Eth-cis	**ctn**
5+1	B	X=Si	$-CH_3$	$-CH_3$	COF-105-Me-Me	**ctn**
5+1	B	X=C	—H	—H	COF-108	**bor**
5+1	B	X=C	$-(CH_2)_5CH_3$	—H	COF-108-nHex-H	**bor**
5+1	B	X=C	$-CH_3$	$-CH_3$	COF-108-Me-Me	**bor**
5+3	B	X=C	N/A	N/A	COF-105-Eth-cis	**ctn**
6+1	C	X=C	—H	—H	COF-202	**ctn**
6+4	C	X=C	—H	—H	COF-212	**ctn**

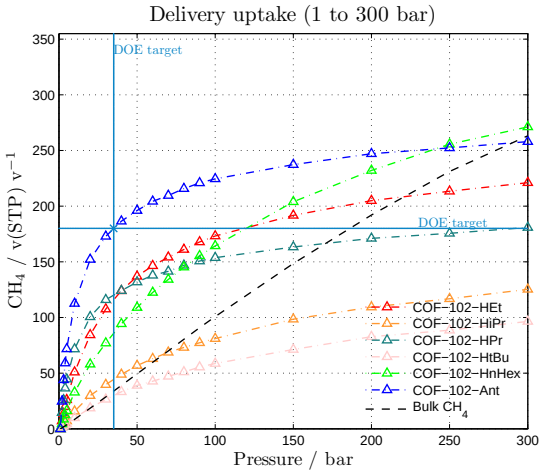
Figure S1: New designed COFs. The inset shows the types of known condensation for COFs. We used these building blocks and condensation modes to design the new COFs.



2.1: Published 2D-COFs



2.2: Published 3D-COFs



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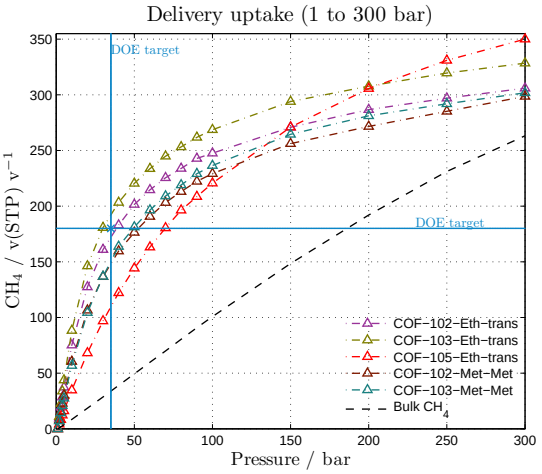

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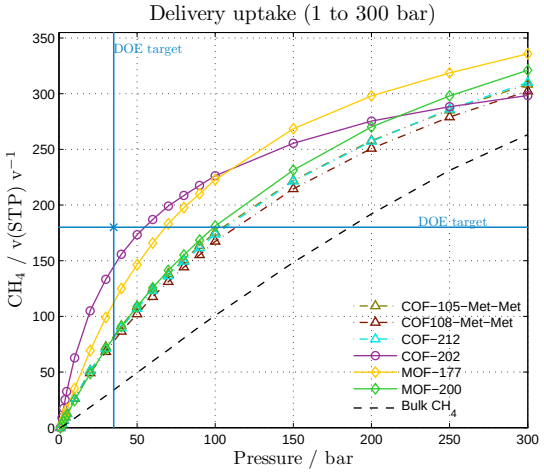

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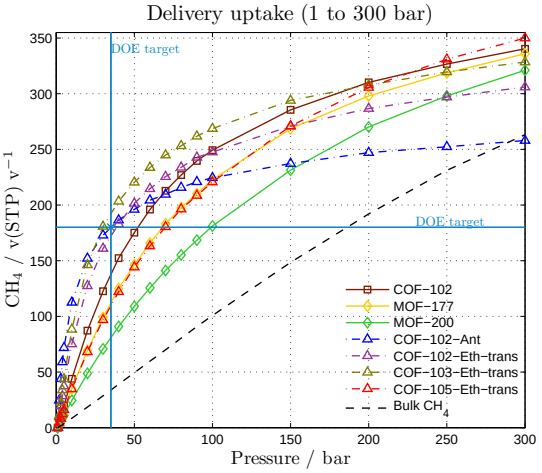
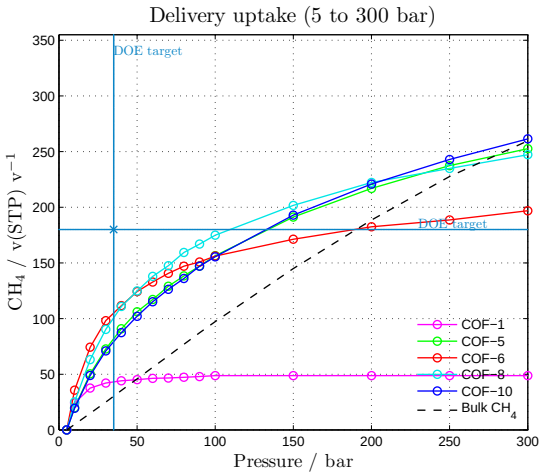
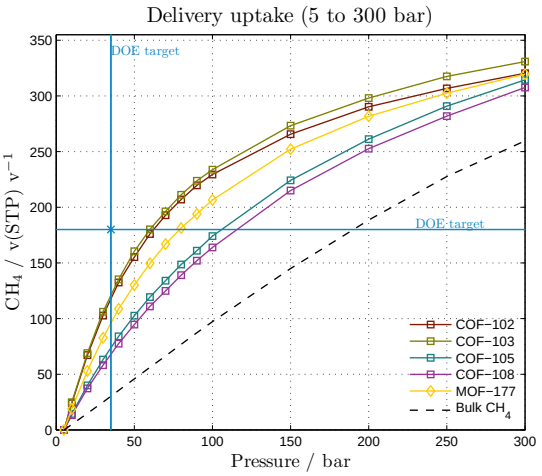


2.6: Best performers

Figure S2: CH_4 delivery amount in v(STP)/v units (1-300 bar)



3.1: Published 2D-COFs



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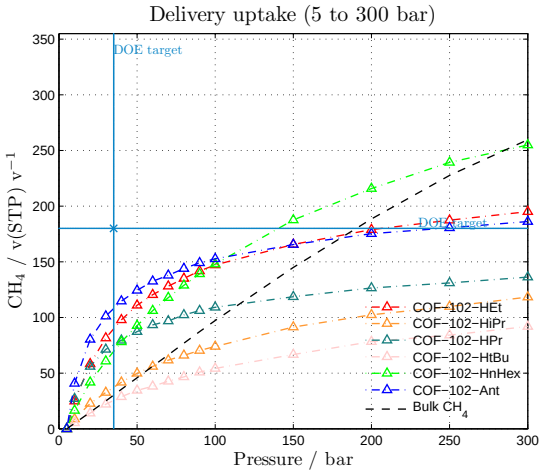

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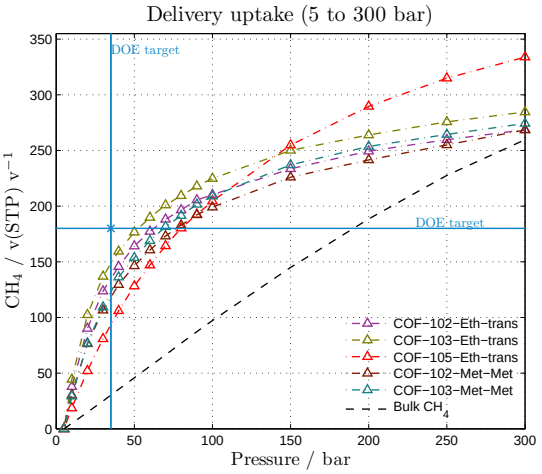

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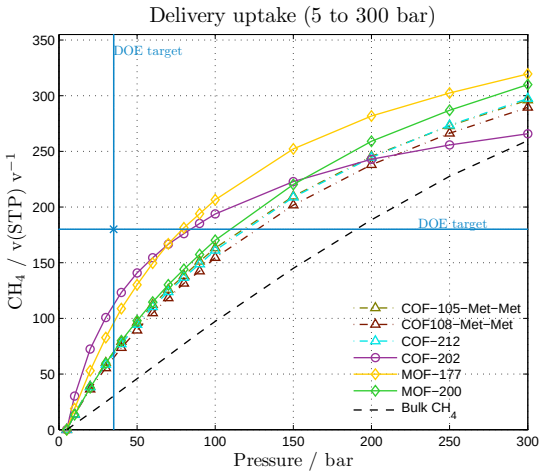

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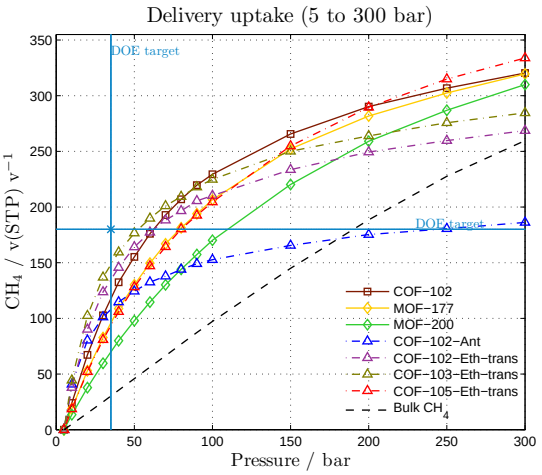
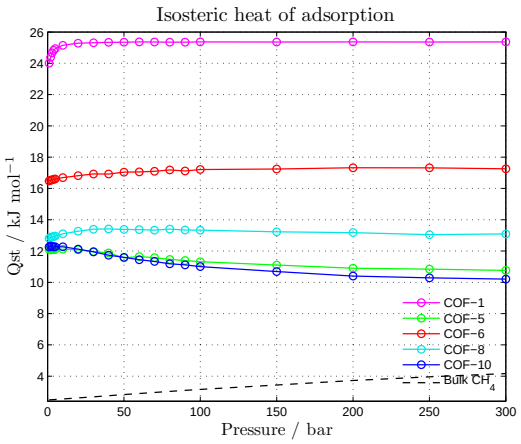


3.6: Best performers

Figure S3: CH_4 delivery amount in v(STP)/v units (5-300 bar)

3 Heat of adsorption (Qst)



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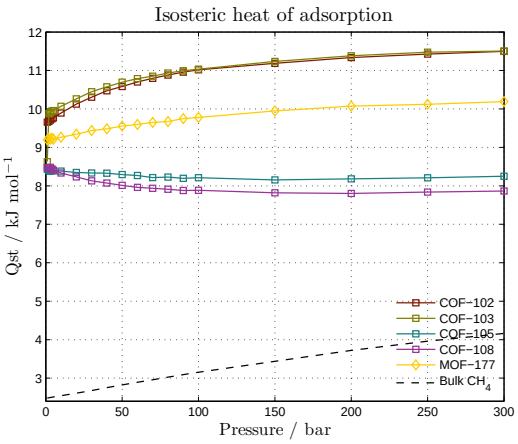

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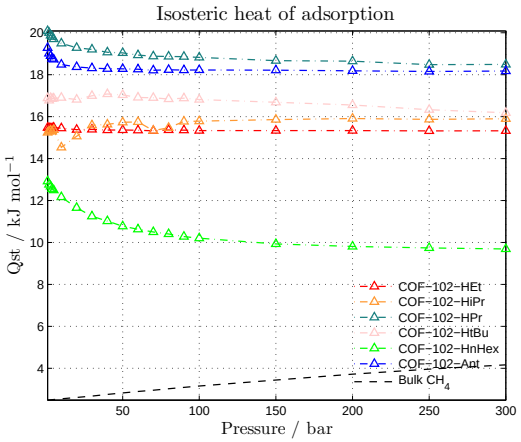

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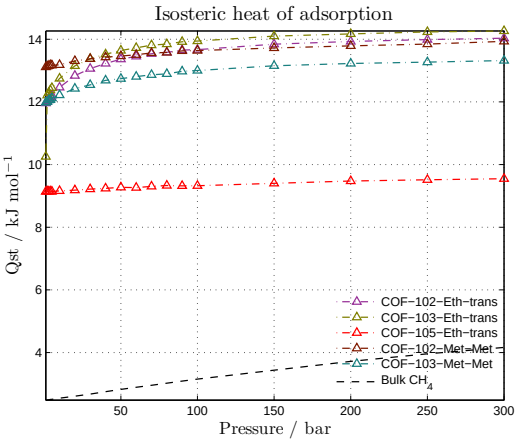

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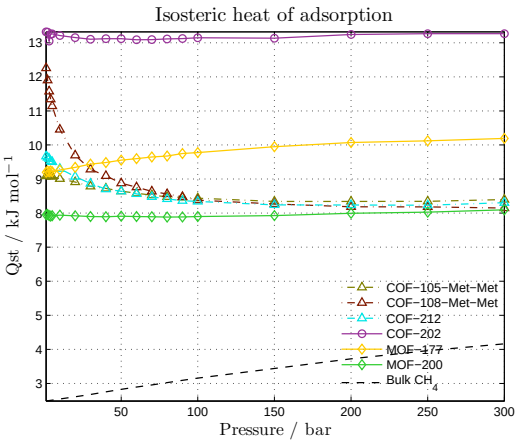

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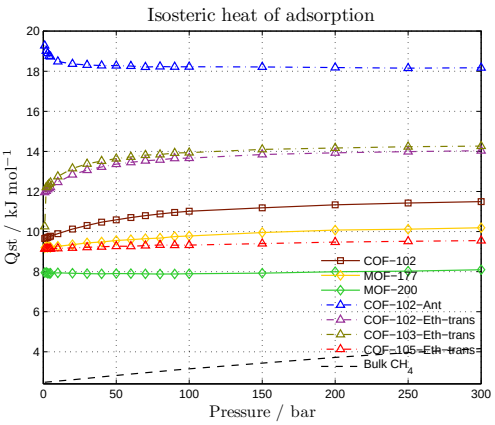


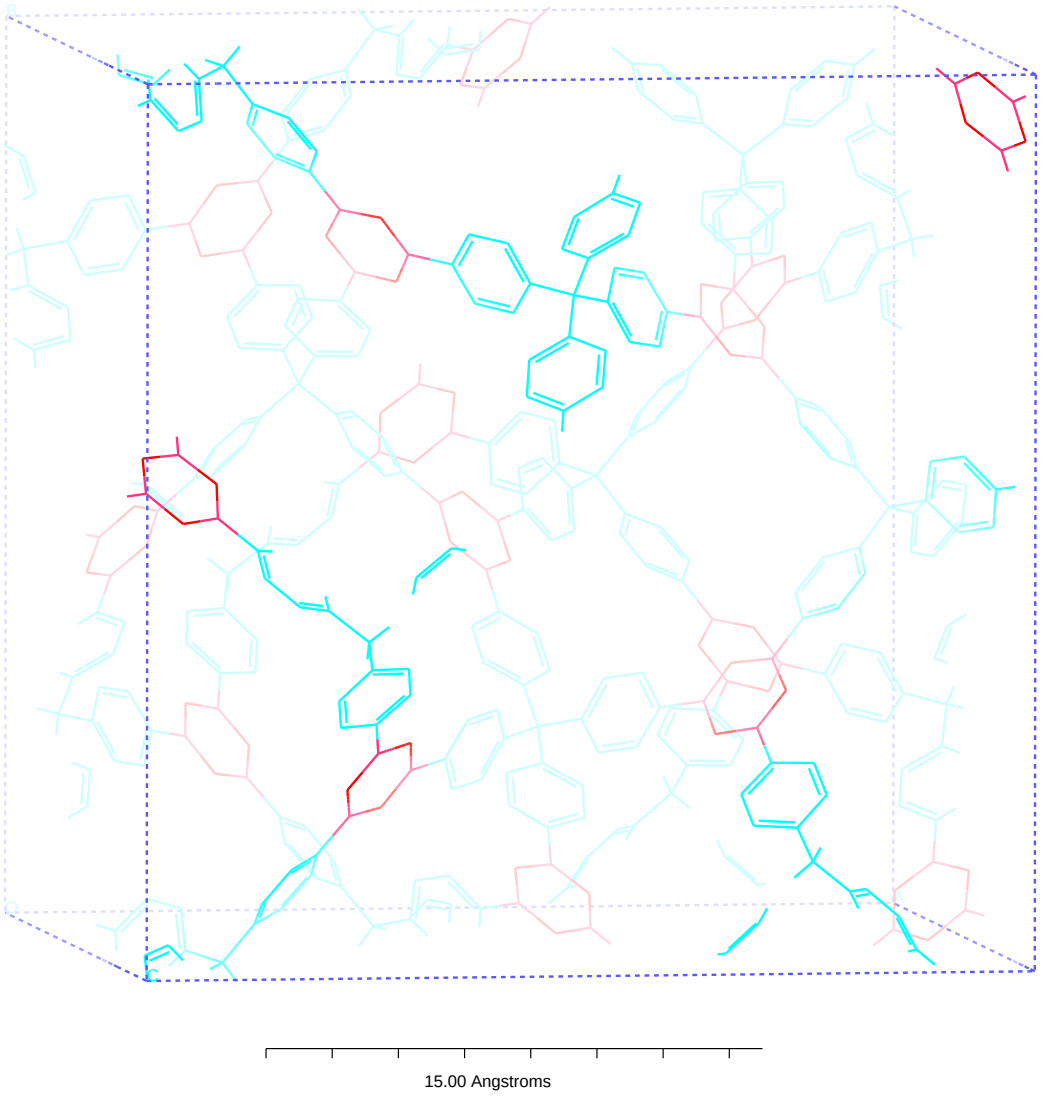
4.6: Best performers

Figure S4: Qst for CH_4 adsorption for the range of 1 to 300 bar.

4 Surface area (S_A), pore volume (V_P) and density (ρ) for the studied frameworks.

Table 1: Properties of COFs. S_A and V_P were estimated from rolling an Ar molecule with diameter of 3.42 Å over the framework's surface.

Compound	S_A / (m^2 g^{-1})	V_P / (cm^3 g^{-1})	ρ / (g cm^{-3})	Topology
COF-1	1230	0.38	0.91	**gra**
COF-5	1520	1.17	0.58	**bnn**
COF-6	1050	0.55	1.03	**bnn**
COF-8	1320	0.87	0.71	**bnn**
COF-10	1830	1.65	0.49	**bnn**
COF-102	4940	1.81	0.42	**ctn**
COF-103	5230	2.05	0.38	**ctn**
COF-105	6450	4.94	0.18	**ctn**
COF-108	6280	5.40	0.17	**ctn**
COF-102-H-Et	3970	0.95	0.64	**ctn**
COF-102-H-iPr	1420	0.63	0.76	**ctn**
COF-102-H-Pr	2590	0.72	0.75	**ctn**
COF-102-H-tBu	900	0.50	0.87	**ctn**
COF-108-H-nHex	5250	2.54	0.31	**bor**
COF-102-Ant	2720	0.75	0.76	**ctn**
COF-102-Eth-trans	4640	1.20	0.57	**ctn**
COF-103-Eth-trans	4920	1.36	0.57	**ctn**
COF-105-Eth-trans	6350	3.62	0.26	**ctn**
COF-102-Met-Met	3500	1.04	0.63	**ctn**
COF-103-Met-Met	3550	1.17	0.57	**ctn**
COF-105-Met-Met	5420	3.72	0.23	**ctn**
COF-108-Met-Met	5340	4.01	0.22	**bor**
COF-202	4500	1.37	0.53	**ctn**
COF-212	6460	4.13	0.21	**ctn**
MOF-177	4800	1.93	0.43	**qom**
MOF-200	5730	4.04	0.22	**qom**



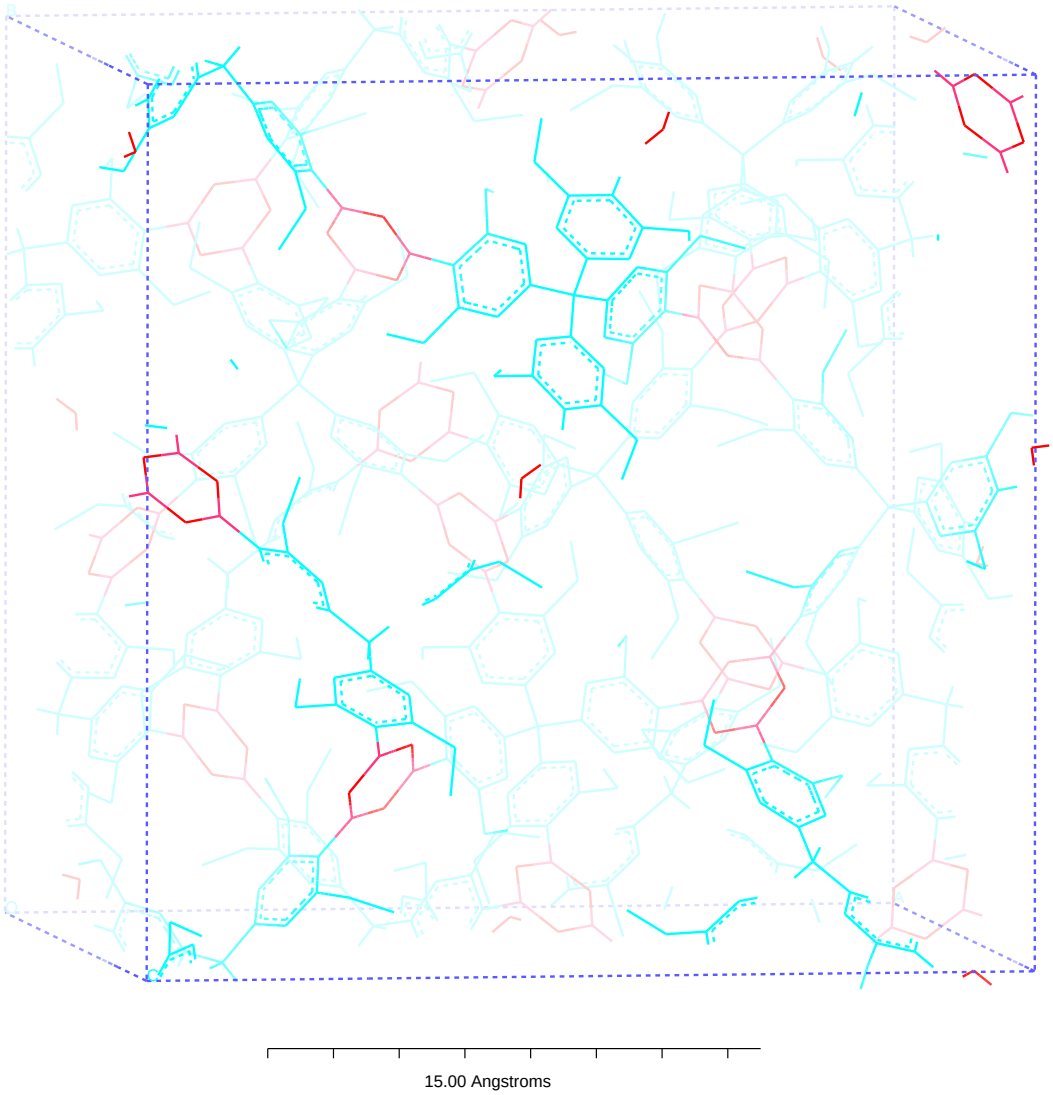
5.1: COF-102

Figure S5: 3D-representation

Name
COF-102

Space group symmetry
I -4 3 d
a = b = c = 27.177 27.177 27.177 A
alpha = betha = gamma = 90

Atom	x	y	z
O1	0.82850	0.74693	0.30298
B1	0.83533	0.71325	0.26216
C1	0.90490	0.76629	0.22758
C2	0.87894	0.72231	0.22630
C3	0.93120	0.69419	0.16049
C4	0.95634	0.73930	0.15960
C5	0.89252	0.68630	0.19272
C6	0.94306	0.77459	0.19484
C7	1.00000	0.75000	0.12500
H1	0.89552	0.79460	0.25352
H2	0.94125	0.66415	0.13717
H3	0.87377	0.65150	0.19176
H4	0.96223	0.80911	0.19660



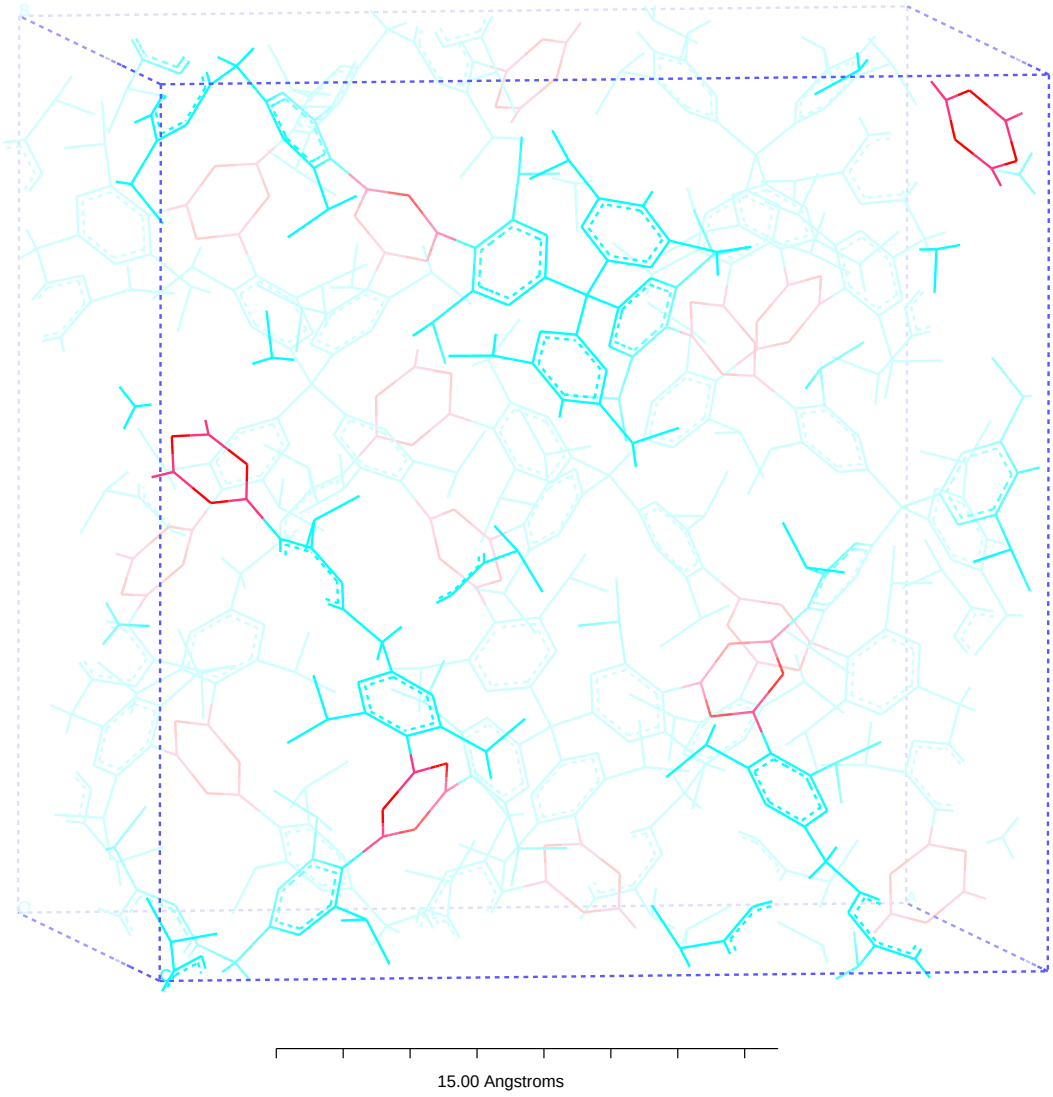
5.2: COF-102-Et-H

Figure S5: 3D-representation

Name
COF-102-Et-H

Space group symmetry
I -4 3 d
a = b = c = 27.190 27.190 27.190 A
 alpha = betha = gamma = 90

Atom	x	y	z
C1	0.37500	0.00000	0.25000
C2	0.31112	0.04591	0.19819
C3	0.33861	0.04238	0.24232
C4	0.32806	0.07808	0.27871
C5	0.29562	0.11798	0.27095
C6	0.27052	0.12130	0.22500
B7	0.23723	0.16369	0.21498
C8	0.27739	0.08429	0.18850
O9	0.19568	0.17363	0.24651
H10	0.17547	0.09495	0.16865
H11	0.17799	0.06639	0.11033
H12	0.19265	0.03217	0.16382
H13	0.31569	0.22849	0.33156
H14	0.35854	0.19516	0.29550
H15	0.30559	0.22132	0.26773
H16	0.34458	0.07507	0.31228
H17	0.31604	0.01922	0.17213
C18	0.25009	0.08307	0.14049
C19	0.29081	0.15525	0.31143
H20	0.25257	0.11864	0.12214
H21	0.26664	0.05672	0.11498
C22	0.19548	0.06826	0.14642
H23	0.25223	0.16372	0.31827
H24	0.30479	0.14081	0.34629
C25	0.31951	0.20316	0.30064



5.3: COF-102-iPr-H

Figure S5: 3D-representation

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Name
COF-102-iPr-H

Space group symmetry
I -4 3 d
a = b = c = 27.085  27.085  27.085  A
 alpha = betha = gamma = 90
Atom            x         y         z
  C1      0.62500   0.50000   0.25000
  C2      0.56088   0.44691   0.29471
  C3      0.58823   0.49138   0.29206
  C4      0.57619   0.52793   0.32734
  C5      0.54239   0.52025   0.36643
  C6      0.51723   0.47390   0.36839
  B7      0.48360   0.46282   0.41038
  C8      0.52445   0.43754   0.33092
  O9      0.44161   0.49390   0.42088
  C10     0.50739   0.60599   0.37974
  H11     0.49928   0.63389   0.40771
  H12     0.52921   0.62327   0.35059
  H13     0.47239   0.59356   0.36400
  C14     0.52659   0.34360   0.33544
  H15     0.50320   0.31077   0.33674
  H16     0.55354   0.33867   0.30593
  H17     0.54609   0.34644   0.37062
  H18     0.44345   0.42068   0.27190
  H19     0.44069   0.35570   0.27746
  H20     0.49041   0.38342   0.24561
  H21     0.57641   0.60375   0.45880
  H22     0.60839   0.59752   0.40238
  H23     0.60382   0.54654   0.44338
  H24     0.59244   0.56174   0.32432
  H25     0.56748   0.42056   0.26853
  C26     0.49468   0.39040   0.32661
  C27     0.53541   0.56177   0.40325
  H28     0.46590   0.38901   0.35475
  C29     0.46563   0.38740   0.27711
  H30     0.51260   0.54992   0.43416
  C31     0.58426   0.57846   0.42838
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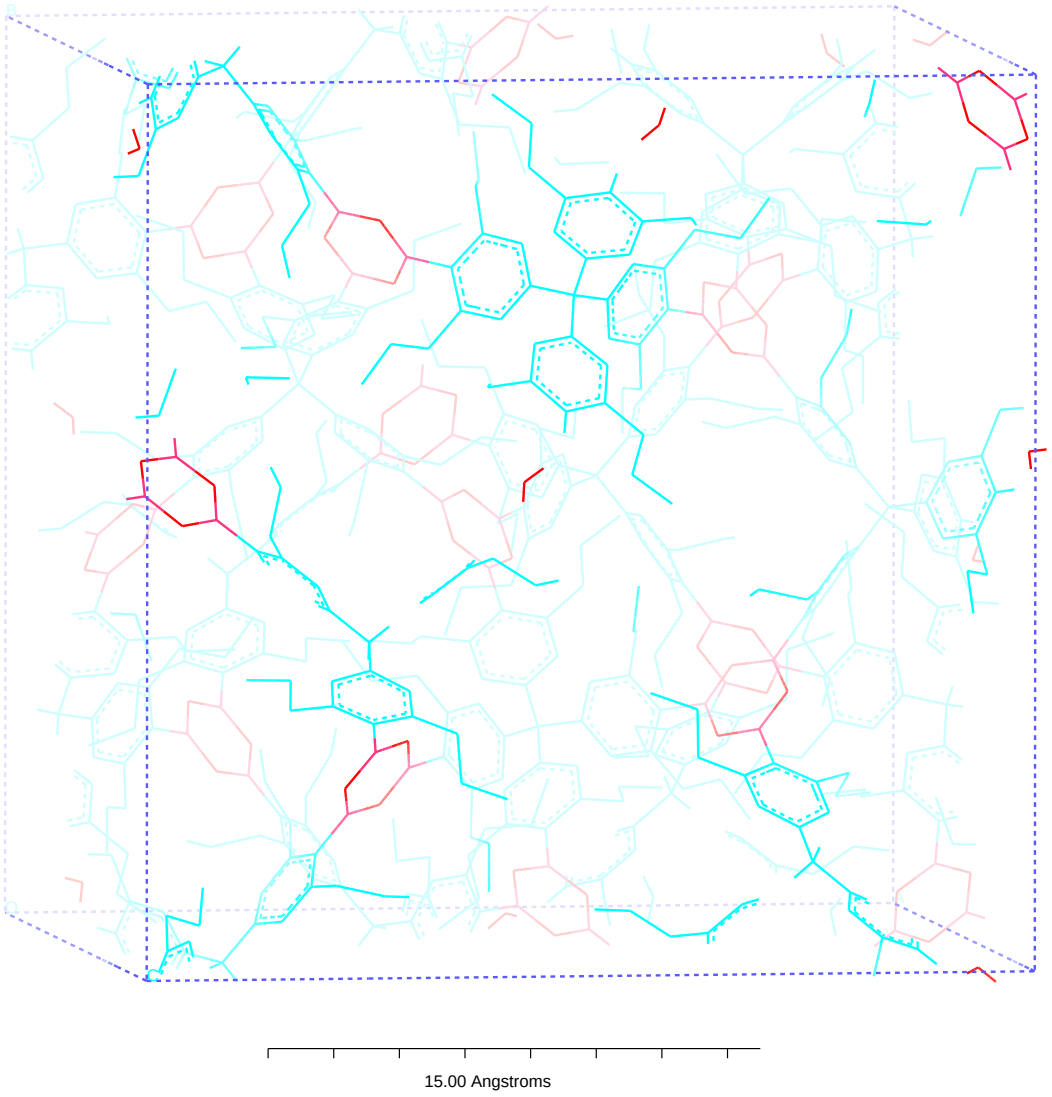

5.4: COF-102-Pr-H

Figure S5: 3D-representation

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Name
COF-102-Pr-H

Space group symmetry
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 alpha = betha = gamma = 90
Atom            x          y          z
  C1      0.62500   0.50000   0.25000
  H2      0.58221   0.43555   0.18606
  H3      0.57787   0.58397   0.22238
  C4      0.51945   0.61858   0.15387
  C5      0.52720   0.43368   0.10717
  H6      0.52837   0.63103   0.11689
  H7      0.54008   0.64308   0.17814
  C8      0.46416   0.62738   0.16495
  H9      0.48766   0.42978   0.10266
  H10     0.53881   0.39979   0.12536
  C11     0.55324   0.43507   0.05639
  H12     0.44128   0.60468   0.14123
  C13     0.44880   0.68149   0.15727
  H14     0.45647   0.61705   0.20298
  H15     0.45741   0.69337   0.11996
  H16     0.46791   0.70530   0.18325
  H17     0.40934   0.68537   0.16296
  C18     0.54394   0.38849   0.02541
  H19     0.59284   0.43888   0.06193
  H20     0.54070   0.46665   0.03519
  H21     0.56232   0.39212  -0.01000
  H22     0.50468   0.38346   0.01904
  H23     0.55841   0.35609   0.04405
  C24     0.56826   0.55599   0.19929
  C25     0.58840   0.50900   0.20835
  C26     0.57075   0.47045   0.17844
  C27     0.53874   0.47789   0.13824
  C28     0.52122   0.52649   0.12877
  B29     0.48781   0.53574   0.08629
  C30     0.53587   0.56614   0.15995
  O31     0.49591   0.57662   0.05357
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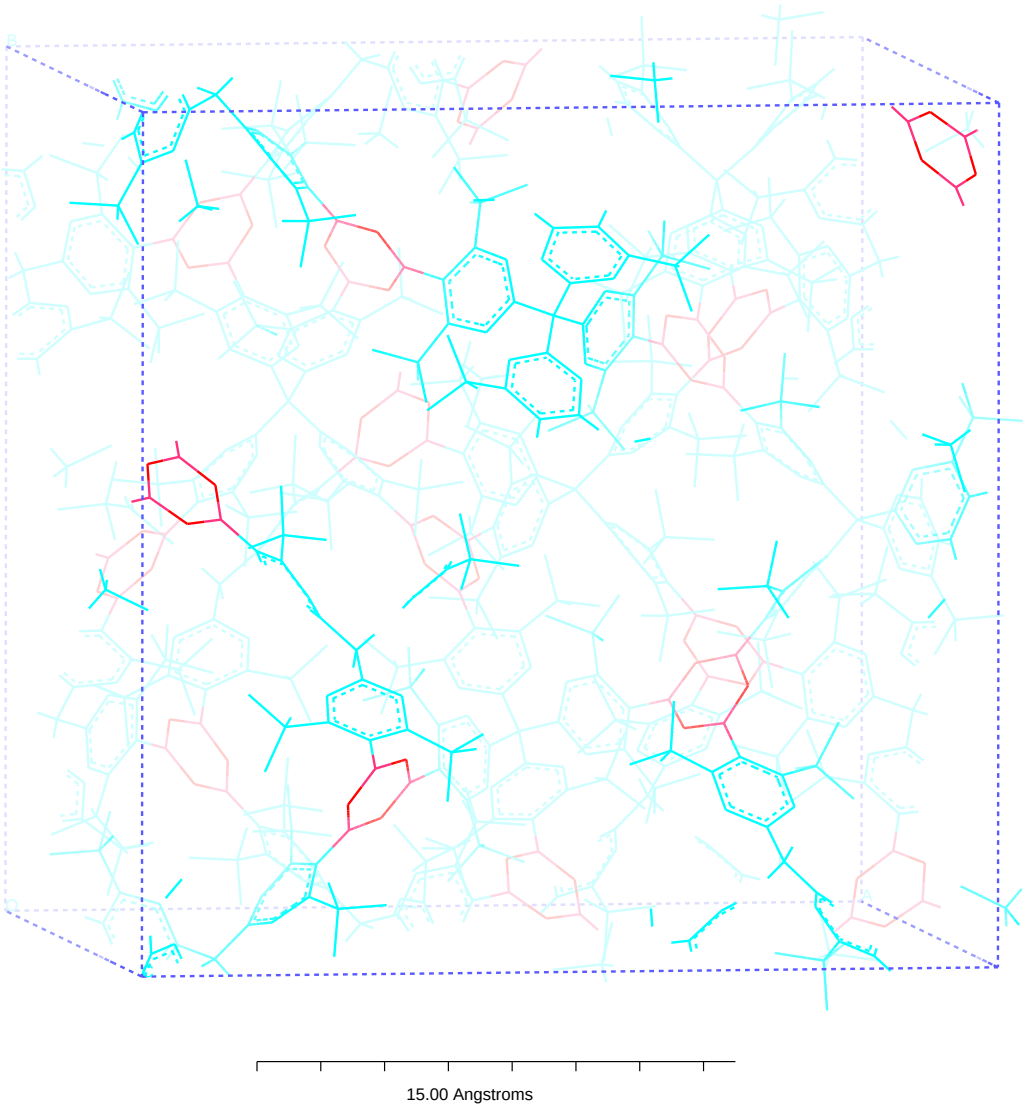


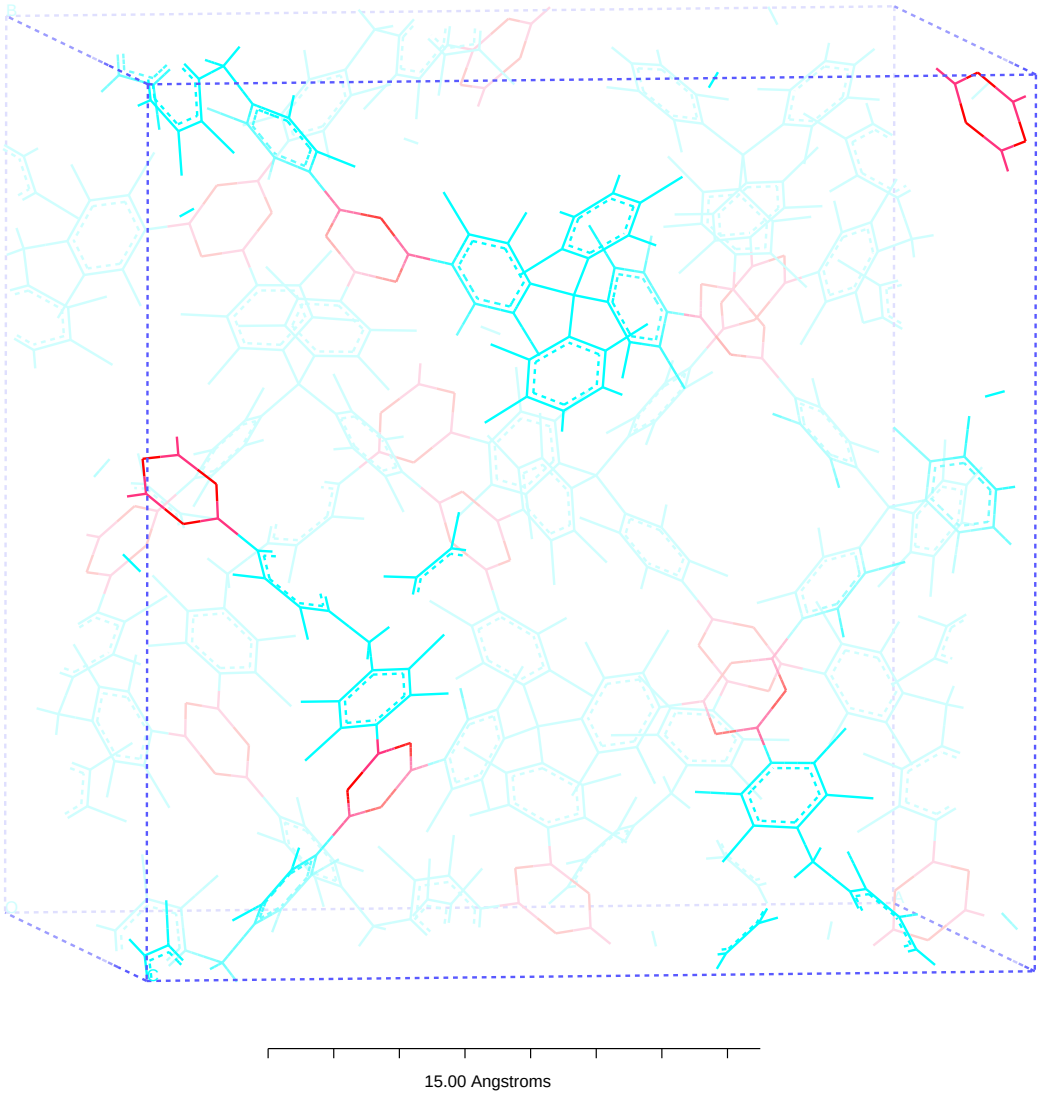
5.5: COF-102-tBu-H

Figure S5: 3D-representation

Name
COF-102-tBu-H

Space group symmetry
I -4 3 d
a = b = c = 27.178 27.178 27.178 A
 alpha = betha = gamma = 90

Atom	x	y	z
C1	0.62500	0.50000	0.25000
C2	0.50042	0.62198	0.18408
C3	0.52586	0.43986	0.10725
H4	0.57783	0.44216	0.18865
H5	0.58372	0.58799	0.22396
C6	0.44311	0.61779	0.18066
H7	0.43084	0.61531	0.14284
H8	0.43009	0.58557	0.20087
H9	0.42406	0.65007	0.19507
C10	0.50822	0.64257	0.23787
H11	0.48522	0.67469	0.24542
H12	0.49905	0.61447	0.26506
H13	0.54577	0.65511	0.24433
C14	0.51856	0.66461	0.15012
H15	0.55862	0.66739	0.15035
H16	0.50668	0.65950	0.11242
H17	0.50362	0.70021	0.16160
C18	0.47480	0.41476	0.11564
H19	0.46077	0.39807	0.08197
H20	0.47612	0.38606	0.14376
H21	0.44781	0.44113	0.12825
C22	0.53296	0.45542	0.05273
H23	0.56725	0.47581	0.04756
H24	0.53202	0.42451	0.02707
H25	0.50267	0.47788	0.04211
C26	0.56427	0.39636	0.11106
H27	0.60171	0.41054	0.10812
H28	0.56083	0.37584	0.14548
H29	0.55967	0.36881	0.08204
C30	0.56790	0.56087	0.20374
C31	0.58788	0.51351	0.20986
C32	0.56704	0.47681	0.18049
C33	0.53346	0.48489	0.14165
C34	0.51192	0.53400	0.13900
B35	0.47587	0.54645	0.09900
C36	0.52638	0.57196	0.17378
O37	0.48366	0.58775	0.06647



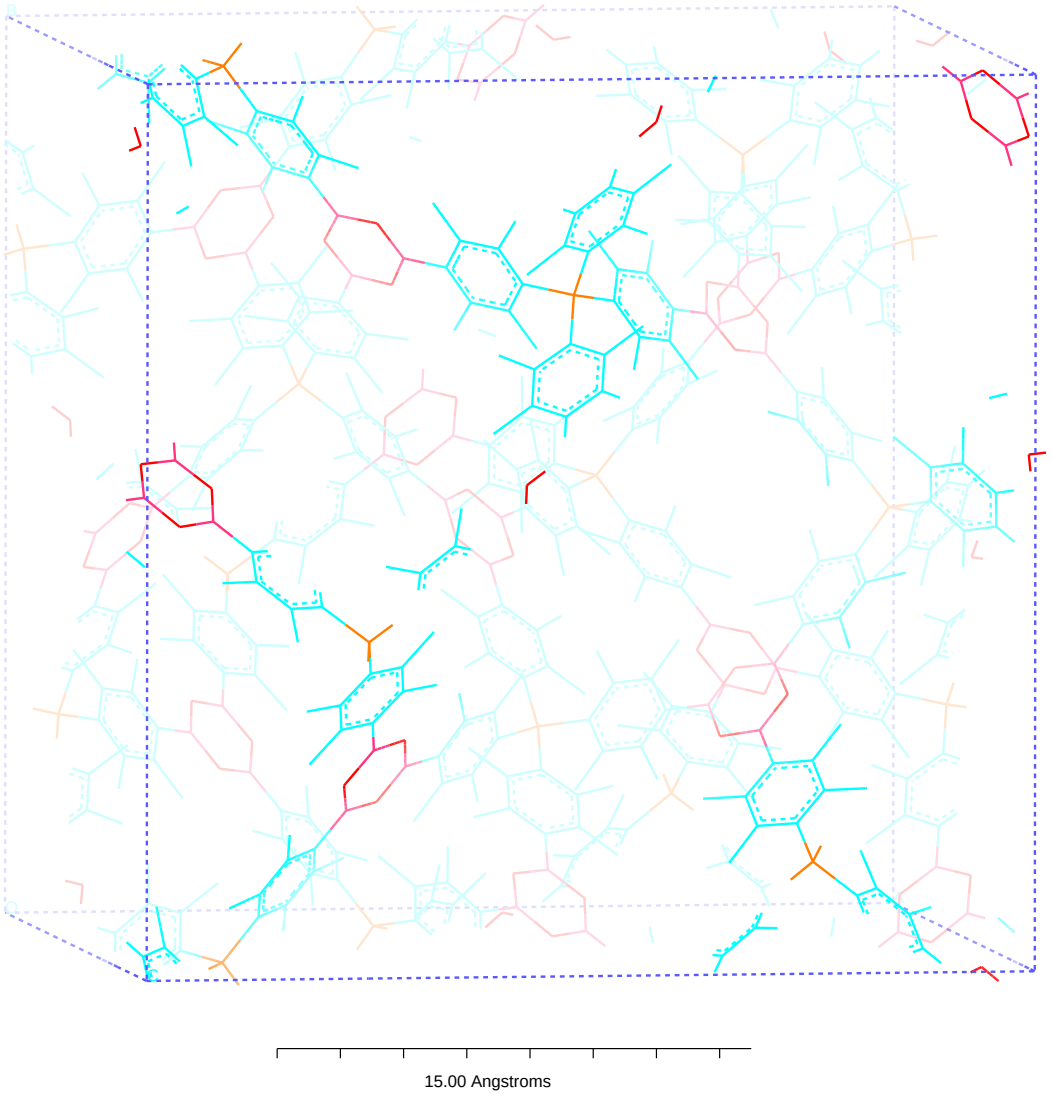
5.7: COF-102-Me-Me

Figure S5: 3D-representation

```
Name
COF-102-Me-Me

Space group symmetry
I -4 3 d
a = b = c = 27.408  27.408  27.408 A
 alpha = betha = gamma = 90
```

Atom	x	y	z
O1	0.19700	0.17173	0.24691
C2	0.00000	0.25000	0.37500
C3	0.06876	0.19417	0.33948
C4	0.04365	0.23929	0.34040
C5	0.05696	0.27460	0.30517
C6	0.09512	0.26629	0.27244
C7	0.12105	0.22229	0.27369
B8	0.16465	0.21323	0.23782
C9	0.10744	0.18627	0.30725
C10	0.02776	0.32244	0.30734
C11	0.05409	0.15687	0.37854
C12	0.13601	0.13886	0.30639
C13	0.10968	0.30443	0.23519
H14	0.03951	0.34933	0.27959
H15	-0.01144	0.31442	0.30101
H16	0.03179	0.33969	0.34378
H17	0.08536	0.14849	0.40289
H18	0.02352	0.16995	0.40171
H19	0.04186	0.12307	0.35985
H20	0.17521	0.14688	0.31272
H21	0.12426	0.11197	0.33414
H22	0.13198	0.12161	0.26995
H23	0.07841	0.31280	0.21084
H24	0.12191	0.33823	0.25388
H25	0.14025	0.29135	0.21202



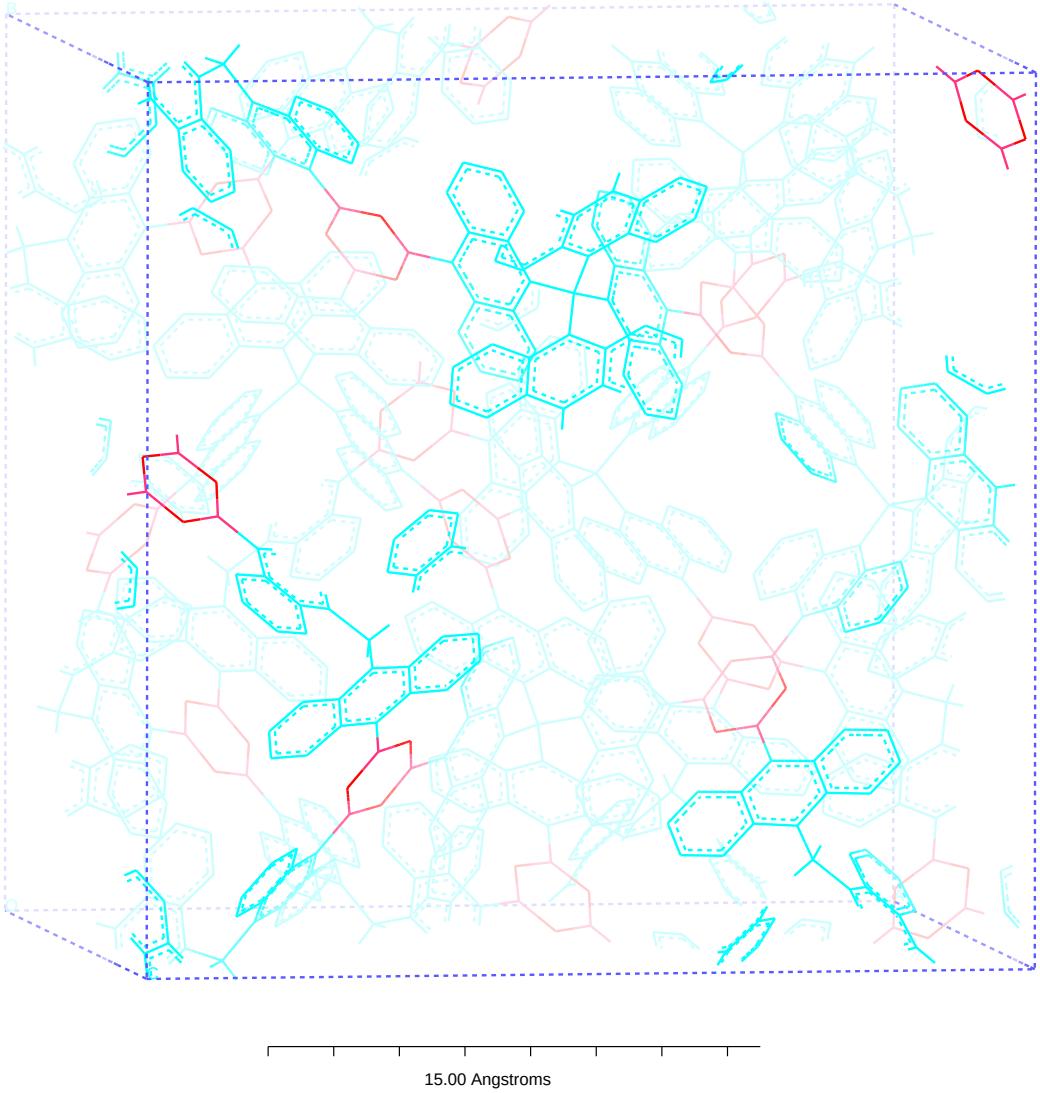
5.8: COF-103-Me-Me

Figure S5: 3D-representation

Name
COF-103-Me-Me

Space group symmetry
I -4 3 d
a = b = c = 28.454 28.454 28.454 A
 alpha = betha = gamma = 90

Atom	x	y	z
C1	0.13828	0.48062	0.45080
C2	0.10068	0.56512	0.59988
C3	0.18314	0.63062	0.58358
C4	0.22075	0.54612	0.43449
H5	0.16194	0.47831	0.42000
H6	0.13978	0.44644	0.46958
H7	0.10197	0.48608	0.43758
H8	0.08362	0.60021	0.60024
H9	0.07245	0.53815	0.59983
H10	0.12166	0.56033	0.63243
H11	0.18164	0.66479	0.56479
H12	0.15949	0.63292	0.61438
H13	0.21945	0.62516	0.59680
H14	0.23781	0.51103	0.43414
H15	0.19977	0.55090	0.40194
H16	0.24898	0.57309	0.43454
Si17	0.25000	0.62500	0.50000
C18	0.17034	0.59070	0.54999
C19	0.19861	0.58591	0.50993
C20	0.18875	0.55021	0.47747
C21	0.15079	0.51989	0.48467
C22	0.12212	0.52496	0.52451
B23	0.07948	0.49102	0.53269
C24	0.13217	0.56062	0.55710
O25	0.04827	0.49979	0.57262

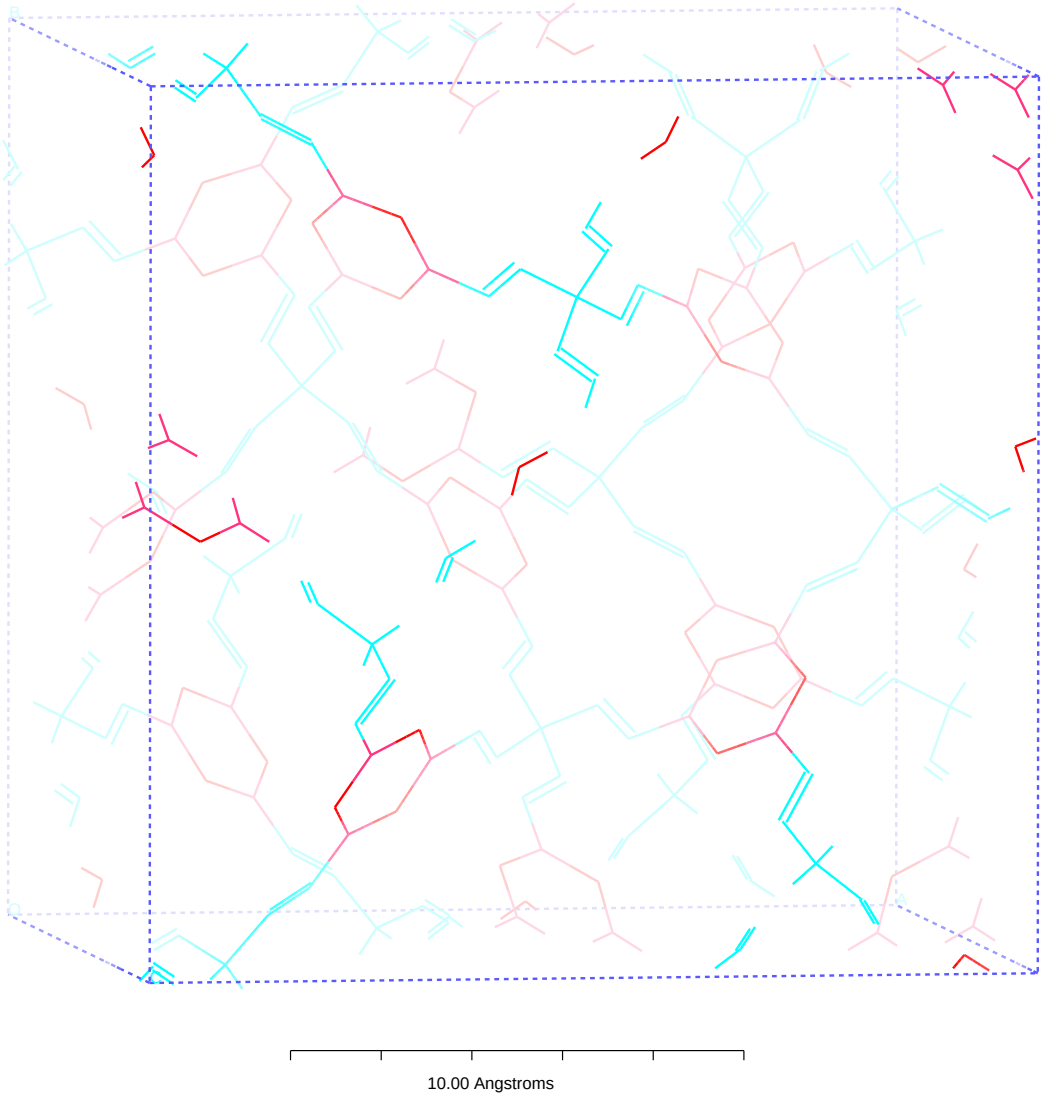


5.9: COF-102-Ant

Figure S5: 3D-representation

```
Name
COF-102-Ant

Space group symmetry
I -4 3 d
a = b = c = 27.821  27.821  27.821 A
 alpha = betha = gamma = 90
Atom            x          y          z
  C1      0.82285   0.54942   0.68100
  C2      0.83516   0.53805   0.73079
  C3      0.80008   0.55693   0.76493
  C4      0.75548   0.57867   0.75152
  C5      0.74858   0.59413   0.70392
  B6      0.71152   0.63670   0.69205
  C7      0.78010   0.57598   0.66850
  O8      0.66988   0.65218   0.72003
  C9      0.87500   0.50000   0.75000
  C10     0.77224   0.58631   0.61978
  H11     0.74036   0.60605   0.60923
  C12     0.80466   0.57106   0.58452
  H13     0.79775   0.57904   0.54707
  C14     0.84600   0.54554   0.59748
  H15     0.87095   0.53384   0.57002
  C16     0.85520   0.53508   0.64578
  H17     0.88736   0.51529   0.65530
  C18     0.72554   0.59596   0.78777
  H19     0.69339   0.61577   0.77825
  C20     0.73475   0.58552   0.83609
  H21     0.70979   0.59722   0.86355
  C22     0.77609   0.56000   0.84905
  H23     0.78300   0.55203   0.88649
  C24     0.80852   0.54475   0.81378
  H25     0.84039   0.52500   0.82433
```

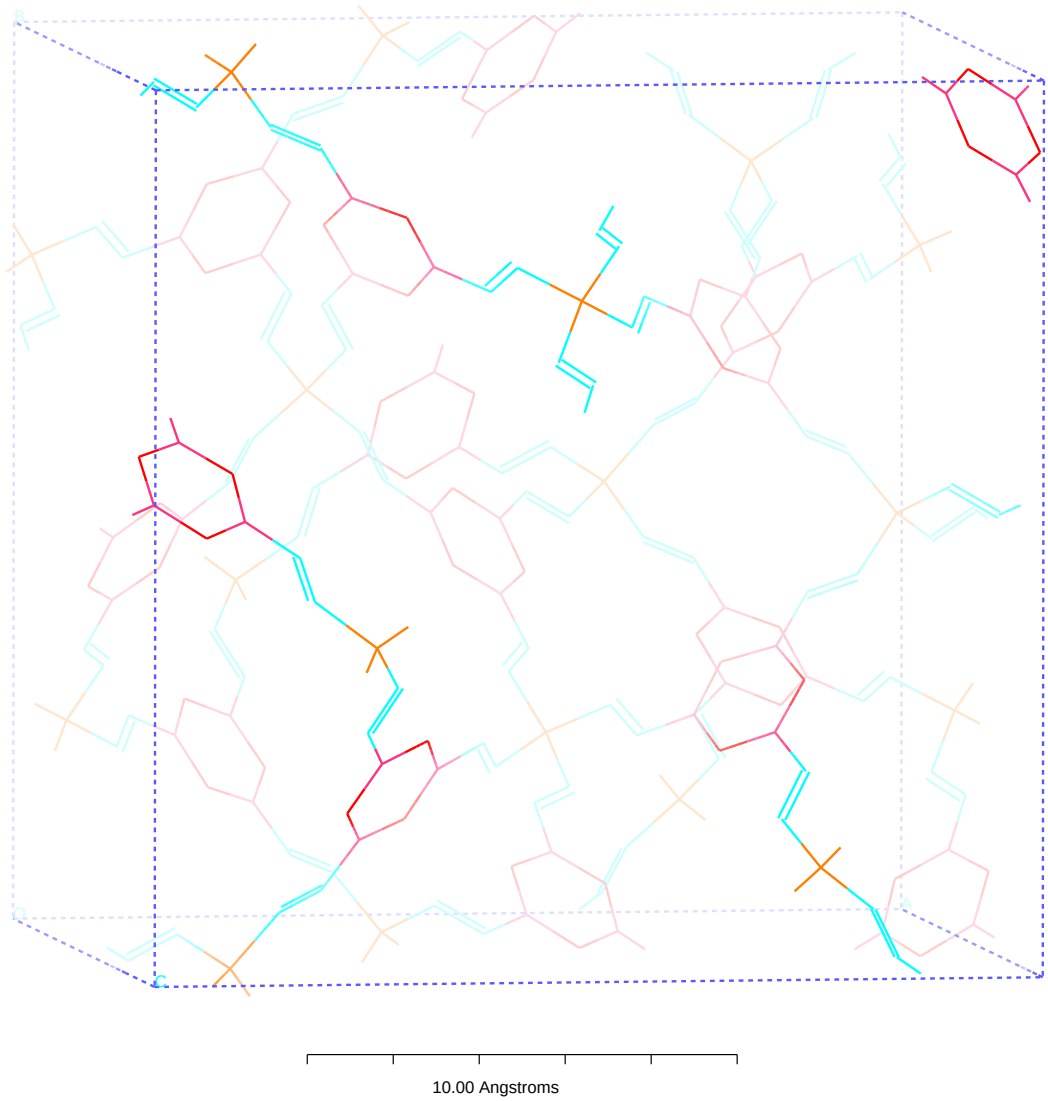


5.10: COF-102-Eth-trans

Figure S5: 3D-representation

```
Name
COF-102-Eth-trans

Space group symmetry
I -4 3 d
a = b = c = 19.779  19.779  19.779 A
 alpha = betha = gamma = 90
Atom            x         y         z
  C1      0.62500   0.50000   0.25000
  B2      0.75957   0.35463   0.22886
  O3      0.73610   0.31890   0.16958
  C4      0.66738   0.44350   0.22168
  C5      0.72293   0.41460   0.25535
  H6      0.65373   0.42238   0.17633
  H7      0.73873   0.43456   0.30031
```

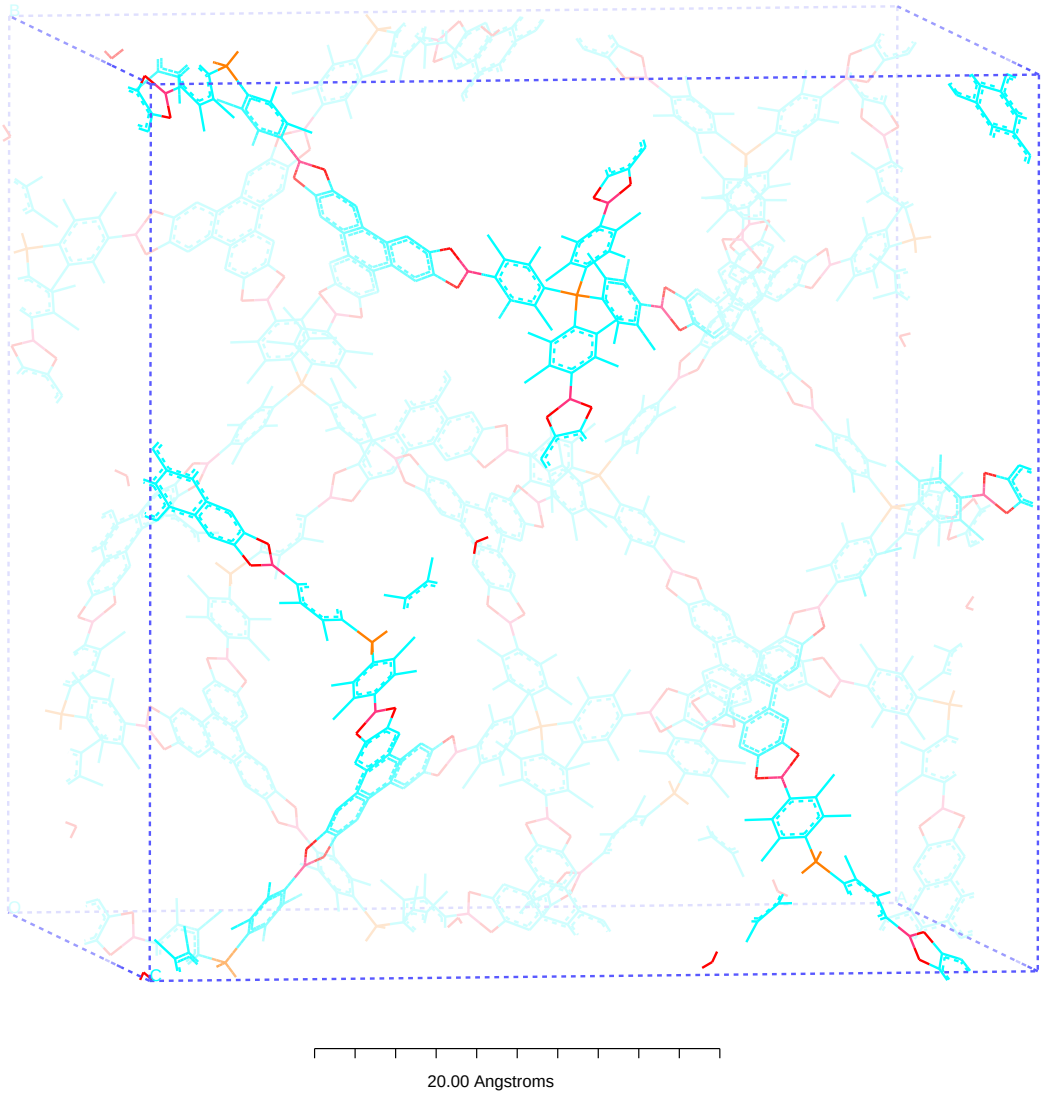


5.11: COF-103-Eth-trans

Figure S5: 3D-representation

```
Name
COF-103-Eth-trans

Space group symmetry
I -4 3 d
a = b = c = 20.250  20.250  20.250 A
 alpha = betha = gamma = 90
Atom            x         y         z
  Si1     0.50000   0.25000   0.62500
  B2      0.47711   0.39586   0.48890
  O3      0.41924   0.43099   0.51157
  C4      0.46984   0.31043   0.57967
  C5      0.50270   0.33728   0.52489
  H6      0.42597   0.33078   0.59423
  H7      0.54616   0.31712   0.50884
```



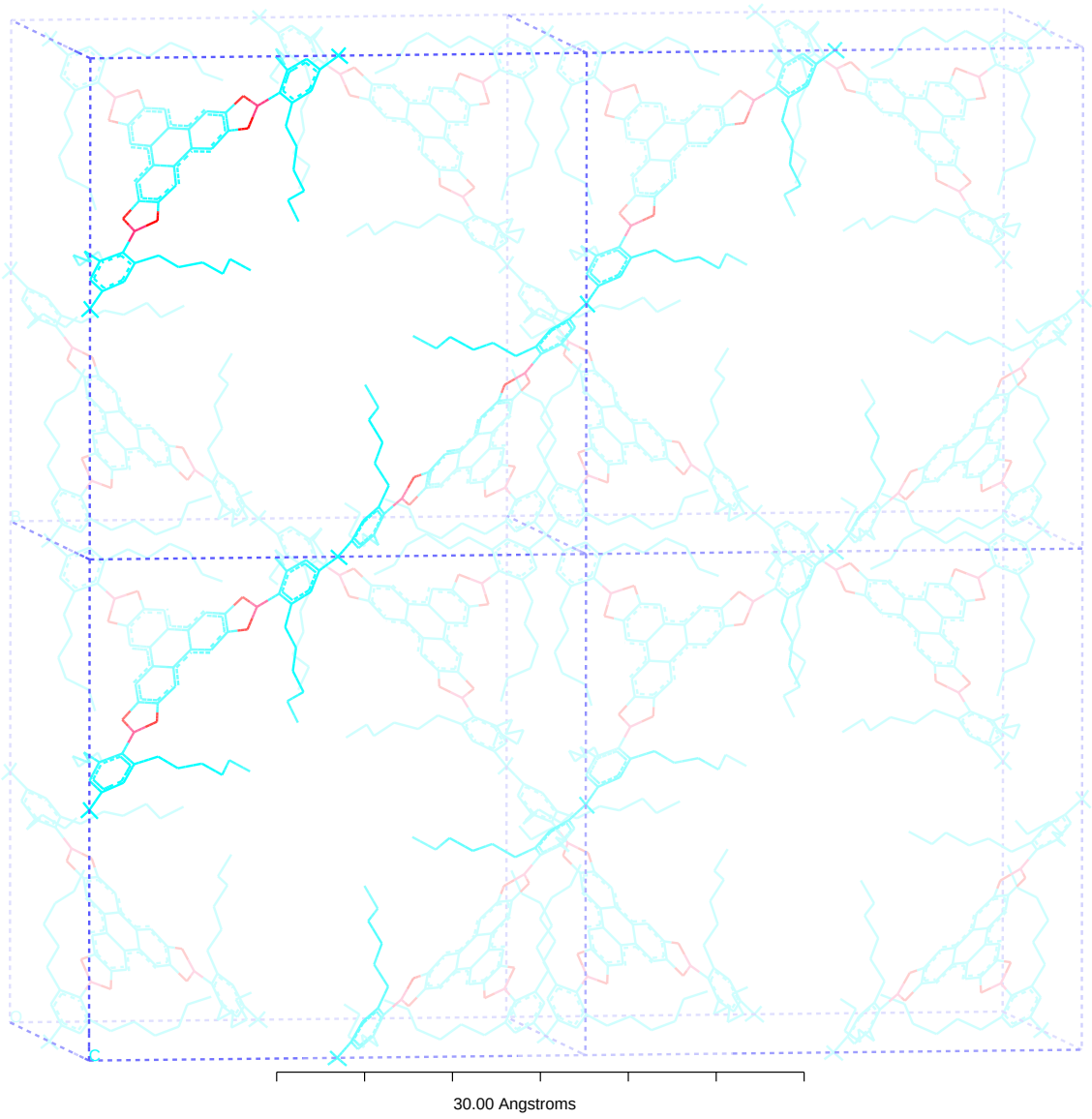
5.12: COF-105-Me-Me

Figure S5: 3D-representation

Name
COF-105-Me-Me

Space group symmetry
I -4 3 d
a = b = c = 44.382 44.382 44.382 A
 alpha = betha = gamma = 90

Atom	x	y	z
Si1	0.37500	0.00000	0.25000
C2	0.21781	0.18335	0.22645
C3	0.23477	0.19174	0.20018
C4	0.22787	0.15826	0.24387
H5	0.21763	0.15114	0.26464
C6	0.25261	0.14166	0.23455
O7	0.26434	0.11672	0.24923
C8	0.26778	0.14873	0.20882
O9	0.29149	0.12931	0.20284
C10	0.25958	0.17328	0.19137
H11	0.27270	0.17680	0.17131
B12	0.28905	0.10906	0.22877
C13	0.35228	0.05035	0.21728
C14	0.34987	0.03288	0.24348
C15	0.32755	0.03978	0.26475
C16	0.30811	0.06410	0.26008
C17	0.31075	0.08180	0.23403
C18	0.33294	0.07478	0.21265
C19	0.28355	0.07305	0.28230
H20	0.28749	0.09649	0.29010
H21	0.26129	0.07200	0.27093
H22	0.28253	0.05838	0.30244
C23	0.32563	0.01996	0.29285
H24	0.30311	0.00913	0.29397
H25	0.32933	0.03390	0.31329
H26	0.34285	0.00179	0.29278
C27	0.33515	0.09429	0.18468
H28	0.35767	0.10512	0.18356
H29	0.31793	0.11246	0.18475
H30	0.33145	0.08035	0.16423
C31	0.37722	0.04150	0.19525
H32	0.39946	0.04266	0.20665
H33	0.37820	0.05618	0.17510
H34	0.37339	0.01804	0.18744



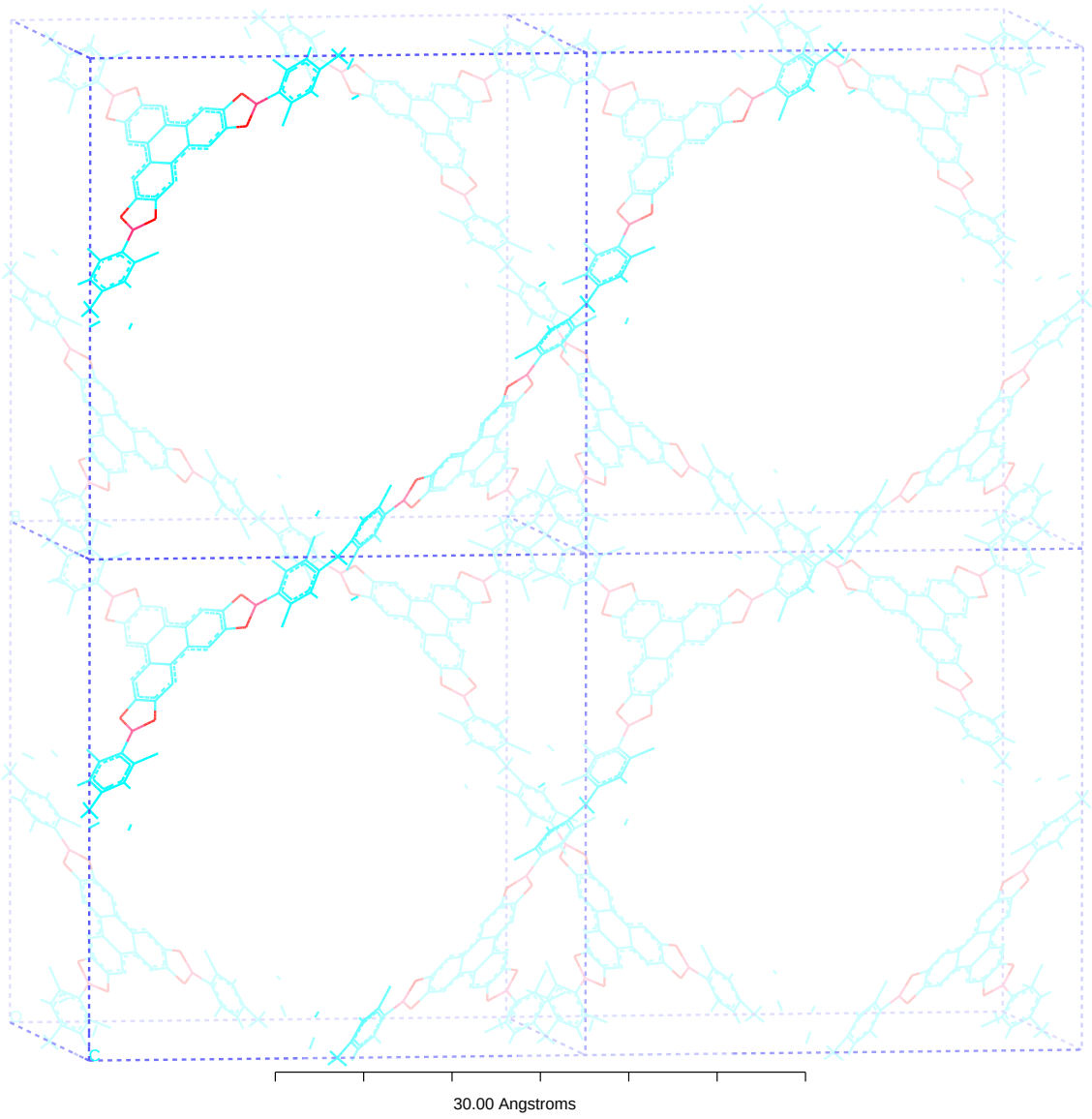
5.14: COF-108-nHex-H

Figure S5: 3D-representation

```
Name
COF-108-nHex-H

Space group symmetry
P -4 3 m
a = b = c = 28.589  28.589  28.589 A
 alpha = betha = gamma = 90
```

Atom	x	y	z
B1	0.64596	0.89336	0.10664
C2	0.60575	0.92134	0.07866
C3	0.58778	0.90432	0.03511
C4	0.55277	0.92945	0.01140
C5	0.53289	0.97056	0.02944
C6	0.77050	0.80583	0.15859
C7	0.70201	0.84295	0.12351
H8	0.73217	0.78277	0.09509
O9	0.66764	0.84984	0.09004
C10	0.73506	0.80743	0.12331
C11	0.50000	0.00000	0.00000
C12	0.01128	0.85980	0.60423
H13	-0.02685	0.86161	0.59649
H14	0.01253	0.85620	0.64272
H15	-0.02221	0.91663	0.54095
C16	1.03135	1.42100	0.18315
H17	1.03056	1.45941	0.17691
H18	1.06830	1.41048	0.18844
C19	0.77297	0.40999	0.99756
C20	0.72916	0.43453	0.97837
H21	0.77875	0.42247	1.03395
H22	0.70261	0.43601	1.00677
H23	0.73773	0.47111	0.96834
C24	0.70803	0.40862	0.93639
H25	0.73349	0.40757	0.90708
H26	0.69933	0.37208	0.94648
H27	0.76718	0.37154	0.99911
C28	0.66356	0.43279	0.91951
H29	0.63680	0.43303	0.94767
H30	0.67130	0.46935	0.90885
H31	0.64924	0.41374	0.88886

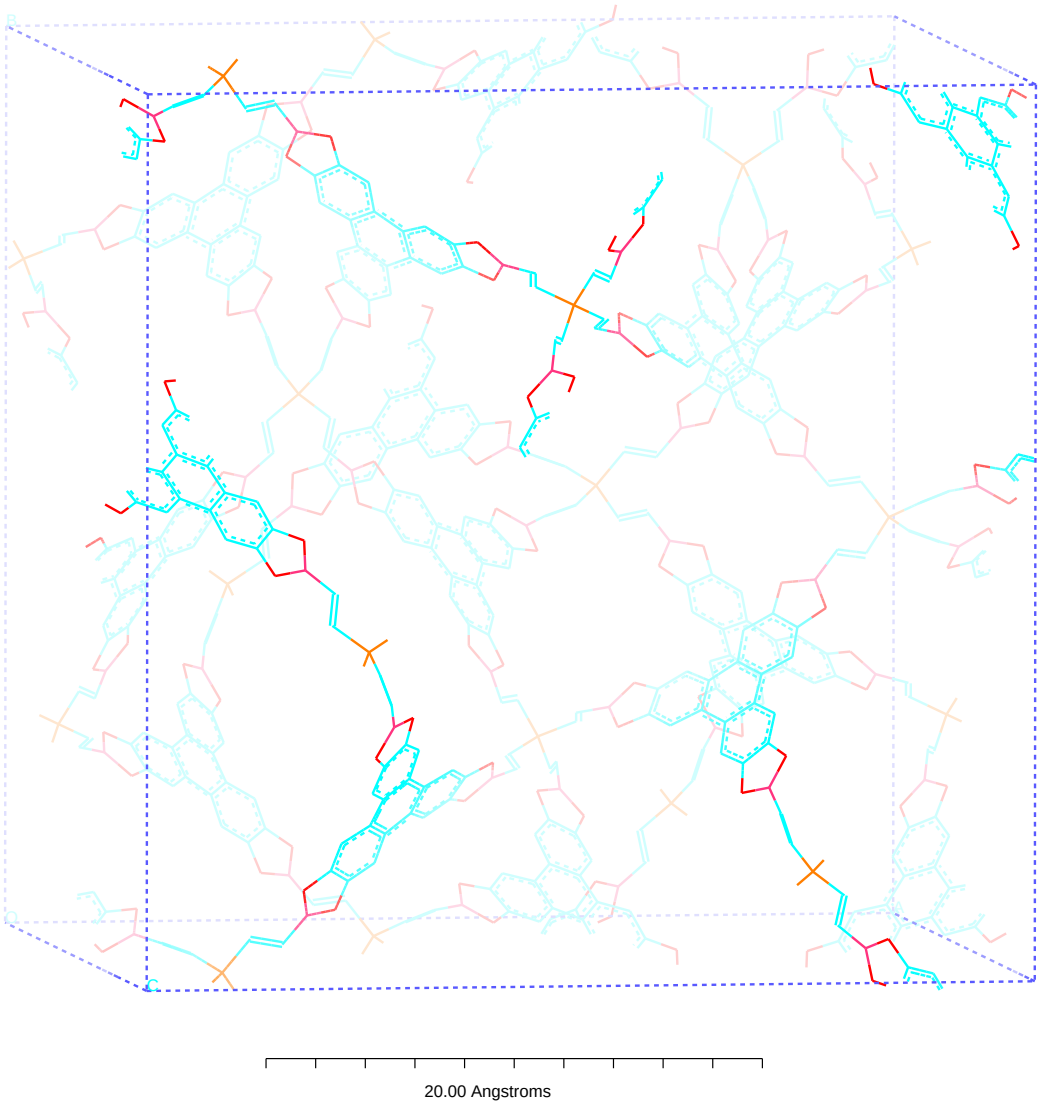


5.15: COF-108-Me-Me

Figure S5: 3D-representation

```
Name
COF-108-Me-Me

Space group symmetry
P -4 3 m
a = b = c = 28.441  28.441  28.441 A
 alpha = betha = gamma = 90
Atom            x         y         z
  B1      0.64886   0.89710   0.10290
  C2      0.60702   0.92264   0.07736
  C3      0.58884   0.90473   0.03528
  C4      0.55309   0.92861   0.01135
  C5      0.53295   0.97038   0.02962
  C6      0.77691   0.81243   0.15180
  C7      0.70726   0.84893   0.11722
  H8      0.73800   0.78882   0.08839
  O9      0.67143   0.85456   0.08457
  C10     0.74101   0.81373   0.11663
  C11     0.50000   0.00000   0.00000
  C12     0.01729   0.85899   0.61001
  H13    -0.01608   0.84640   0.59442
  H14     0.01147   0.86392   0.64830
  H15     0.04413   0.83109   0.60490
  C16    -0.03469   0.91013   0.53223
  H17    -0.06178   0.90786   0.56025
  H18    -0.02892   0.87483   0.51658
  H19    -0.04850   0.93351   0.50416
```

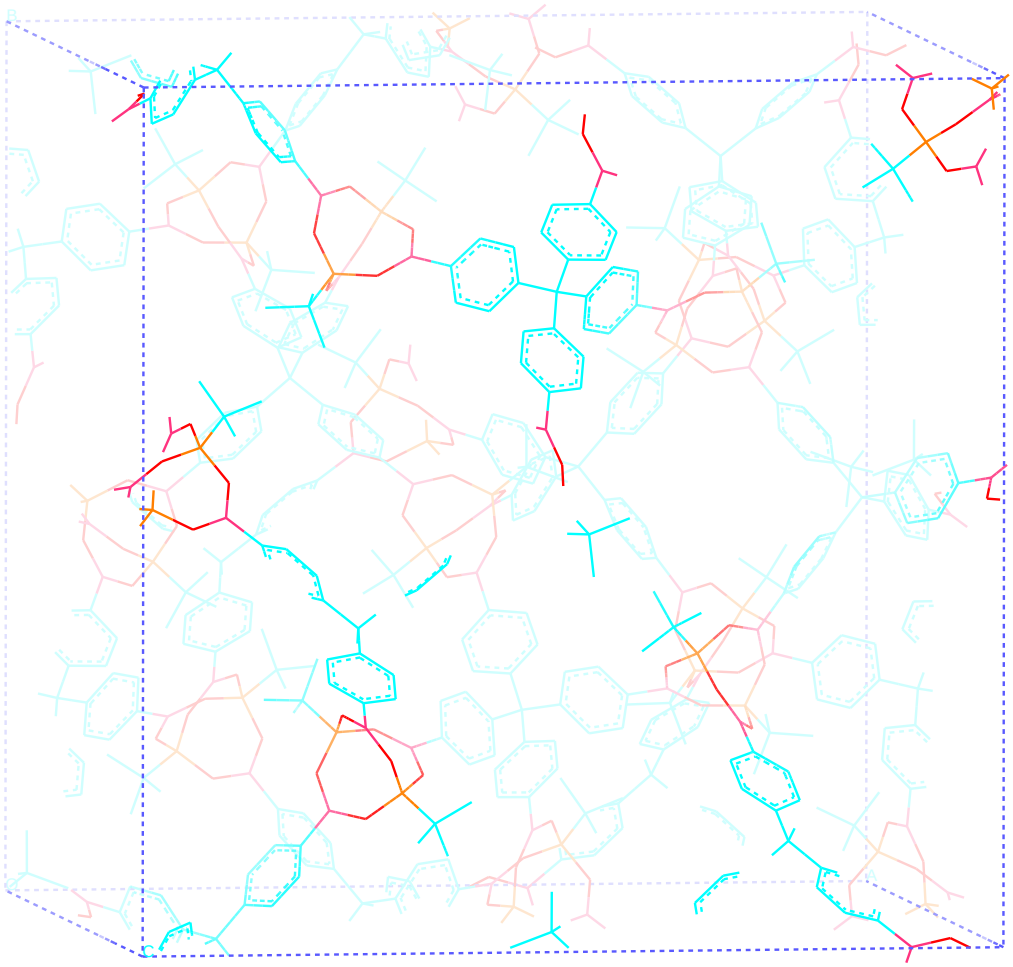


5.16: COF-105-Eth-trans

Figure S5: 3D-representation

```
Name
COF-105-Eth-trans

Space group symmetry
I -4 3 d
a = b = c = 35.925  35.925  35.925 A
 alpha = betha = gamma = 90
Atom            x         y         z
  C1      0.21281   0.20244   0.15966
  C2      0.18156   0.22454   0.17137
  C3      0.22048   0.24370   0.10564
  O4      0.23430   0.25627   0.07309
  C5      0.19296   0.26722   0.11898
  C6      0.17354   0.25807   0.15143
  H7      0.15378   0.27661   0.15964
  C8      0.23080   0.21192   0.12549
  H9      0.25131   0.19622   0.11389
  O10     0.18863   0.29710   0.09647
  B11     0.21457   0.29056   0.06656
  Si12    0.25000   0.37500   0.00000
  C13     0.23661   0.34996   0.03620
  C14     0.22094   0.31430   0.03344
  H15     0.24032   0.36123   0.06209
  H16     0.21538   0.30269   0.00809
```

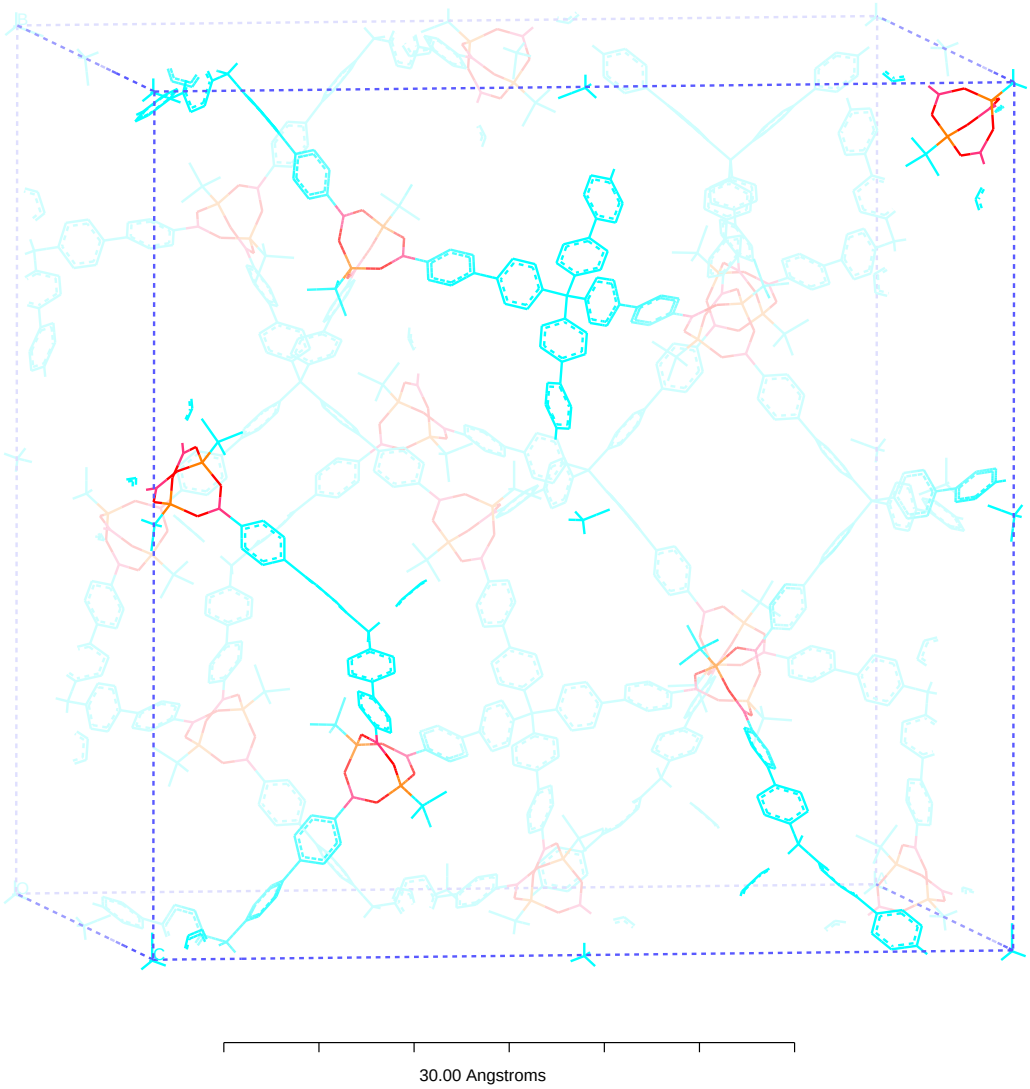


5.17: COF-202

Figure S5: 3D-representation

```
Name
COF-202

Space group symmetry
I -4 3 d
a = b = c = 29.927  29.927  29.927 A
 alpha = betha = gamma = 90
Atom            x         y         z
  C1      0.92551   0.69796   0.21730
  C2      0.88866   0.72727   0.21939
  C3      0.88889   0.76530   0.19154
  C4      0.92449   0.77333   0.16199
  C5      0.96088   0.74313   0.15750
  C6      0.96063   0.70584   0.18707
  H7      0.86329   0.78795   0.19268
  H8      0.92703   0.67032   0.23736
  H9      0.98650   0.68350   0.18658
  H10     0.92318   0.80226   0.14407
  C11     0.37500   0.00000   0.25000
  Si12    0.73964   0.73964   0.73964
  C13     0.82206   0.77388   0.75464
  O14     0.74019   0.76139   0.69121
  B15     0.71851   0.74997   0.64964
  O16     0.68931   0.71237   0.64158
  C17     0.66633   0.62131   0.59801
  H18     0.83675   0.74044   0.75434
  H19     0.84331   0.79501   0.77549
  H20     0.67868   0.64878   0.57734
  H21     0.69495   0.60130   0.60870
  H22     0.64546   0.60015   0.57679
  Si23    0.67243   0.67243   0.67243
  C24     0.63895   0.63895   0.63895
  C25     0.77313   0.77313   0.77313
  H26     0.82331   0.78719   0.72066
```



5.18: COF-212

Figure S5: 3D-representation

```
Name
COF-212

Space group symmetry
I -4 3 d
a = b = c = 45.779  45.779  45.779 A
 alpha = betha = gamma = 90
Atom            x          y          z
  B1      0.83185   0.71326   0.26588
  O2      0.83698   0.69455   0.29078
  Si3     0.81669   0.68331   0.31669
  C4      0.83857   0.66143   0.33857
  C5      0.85418   0.73759   0.22158
  C6      0.90523   0.72925   0.20740
  C7      0.90817   0.71056   0.23184
  C8      0.85707   0.71881   0.24595
  C9      0.87782   0.74271   0.20265
  Si10    0.77296   0.72704   0.27296
  C11     0.75108   0.74892   0.25108
  O12     0.80449   0.72709   0.25838
  C13     0.88451   0.70543   0.25078
  C14     0.94537   0.71082   0.17669
  C15     0.92882   0.73425   0.18808
  C16     0.93654   0.76288   0.17947
  C17     0.95940   0.76773   0.15955
  C18     0.97528   0.74434   0.14673
  C19     0.96823   0.71584   0.15680
  C20     0.76371   0.78068   0.24986
  C21     0.85068   0.63508   0.32045
  H22     0.88766   0.69174   0.26815
  H23     0.92769   0.70056   0.23620
  H24     0.92564   0.78056   0.18776
  H25     0.83480   0.74780   0.21719
  H26     0.87470   0.75627   0.18514
  H27     0.94081   0.68974   0.18262
  H28     0.97982   0.69813   0.14972
  H29     0.96438   0.78888   0.15443
  H30     0.86392   0.64249   0.30202
  H31     0.83301   0.62146   0.31194
  H32     0.86451   0.62119   0.33409
  H33     0.78576   0.78097   0.24071
  H34     0.75005   0.79459   0.23610
  H35     0.76451   0.79061   0.27156
  C36     1.00000   0.75000   0.12500
```

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